



Full wwPDB X-ray Structure Validation Report i

Aug 21, 2020 – 06:55 PM BST

PDB ID : 6QL4
Title : Crystal structure of nucleotide-free Mgm1
Authors : Faelber, K.; Dietrich, L.; Noel, J.K.; Wollweber, F.; Pfitzner, A.-K.; Muehleip, A.; Sanchez, R.; Kudryashev, M.; Chiaruttin, N.; Lilie, H.; Schlegel, J.; Rosenbaum, E.; Hessenberger, M.; Matthaeus, C.; Noe, F.; Roux, A.; vanderLaan, M.; Kuehlbrandt, W.; Daumke, O.
Deposited on : 2019-01-31
Resolution : 3.60 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the i symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.1.3
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

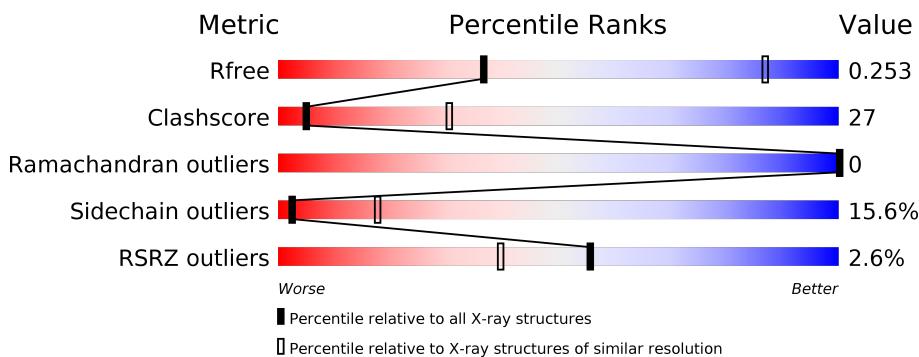
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

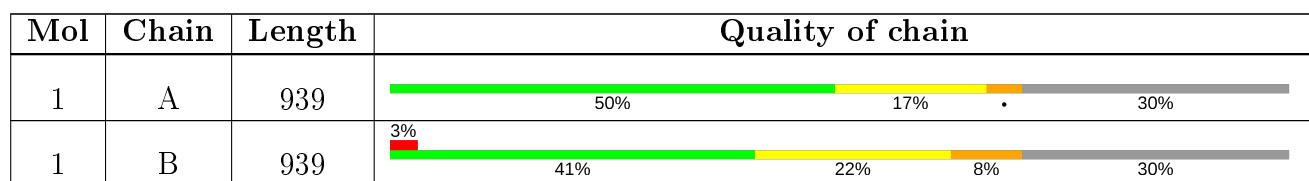
The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	1001	-	-	-	X

2 Entry composition [\(i\)](#)

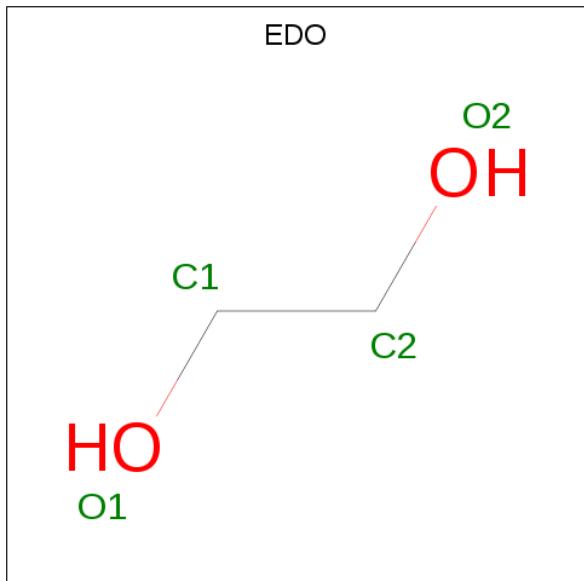
There are 2 unique types of molecules in this entry. The entry contains 10330 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative mitochondrial dynamin protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	Se	0	0	0
			5163	3249	914	983	5	12			
1	B	660	Total	C	N	O	S	Se	0	0	0
			5159	3247	911	984	5	12			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

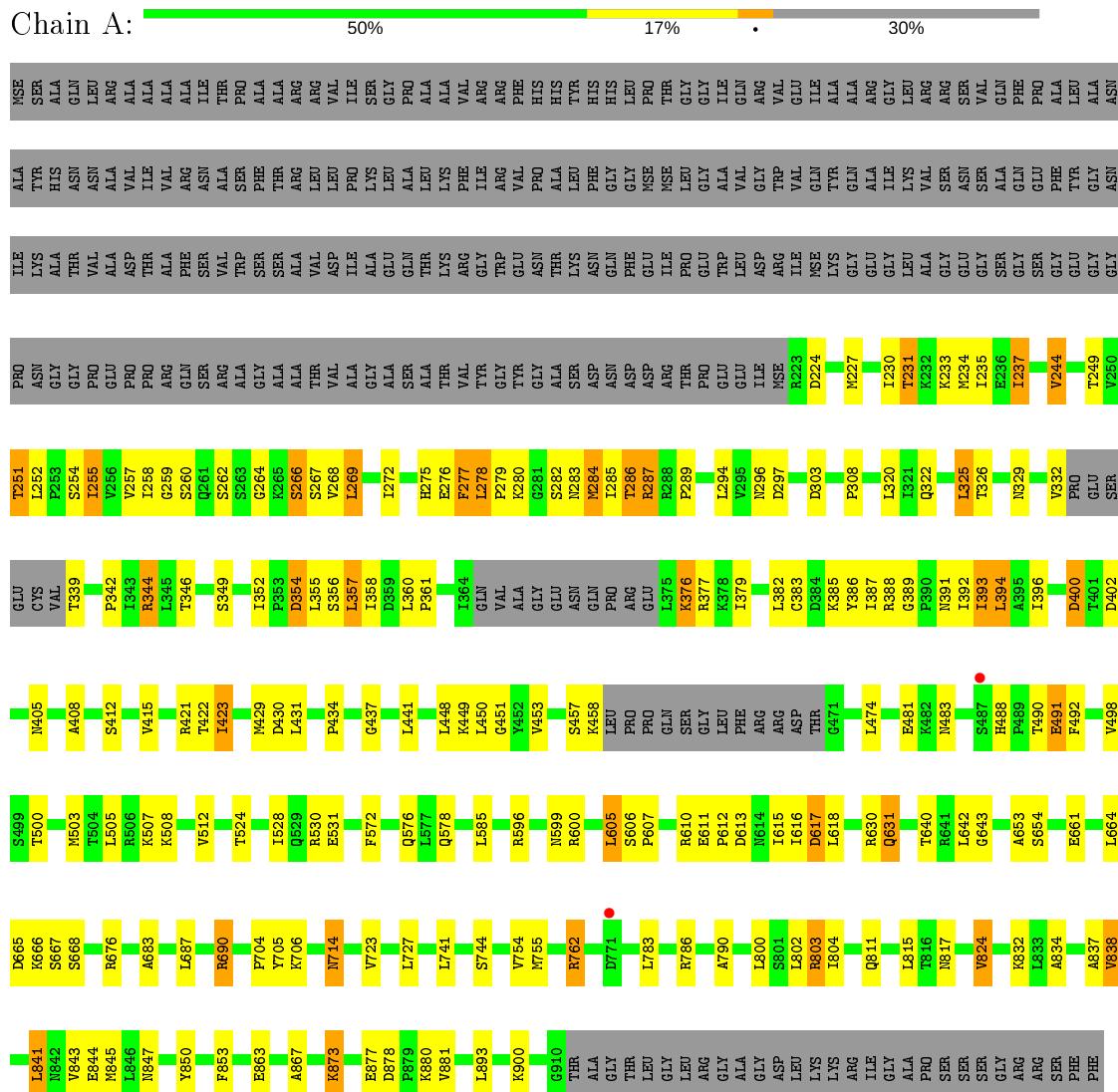


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

3 Residue-property plots

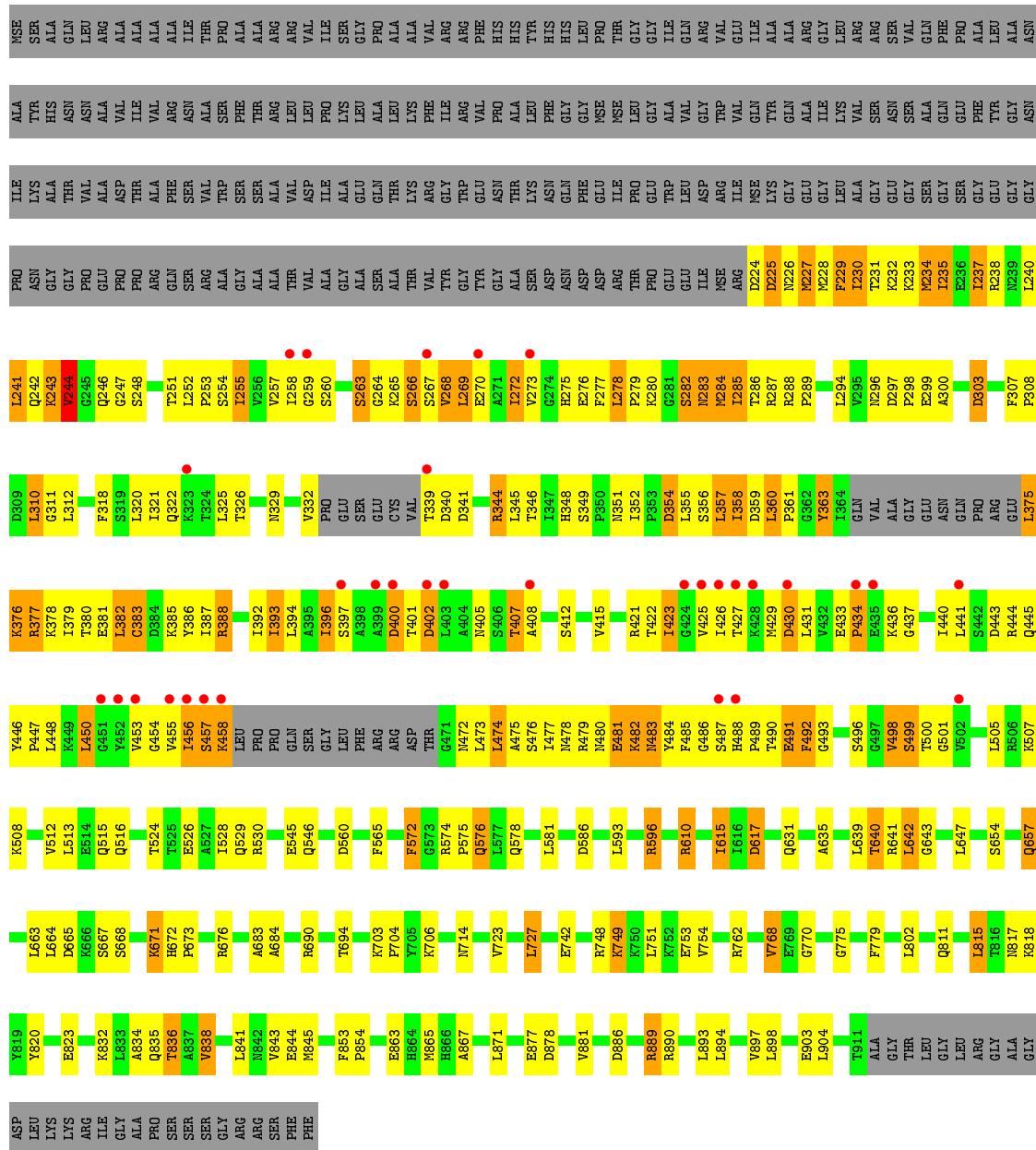
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Putative mitochondrial dynamin protein



- Molecule 1: Putative mitochondrial dynamin protein





4 Data and refinement statistics i

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	147.40 Å 147.40 Å 344.68 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 3.60 49.13 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.13-3.60) 99.8 (49.13-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.61 (at 3.57 Å)	Xtriage
Refinement program	PHENIX	Depositor
R , R_{free}	0.243 , 0.252 0.244 , 0.253	Depositor DCC
R_{free} test set	2242 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	113.6	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10330	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.27	0/5237	0.47	2/7053 (0.0%)
1	B	0.42	1/5233 (0.0%)	0.60	4/7049 (0.1%)
All	All	0.36	1/10470 (0.0%)	0.54	6/14102 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	PRO	C-N	-9.01	1.13	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	MSE	CB-CG-SE	-6.17	94.19	112.70
1	B	815	LEU	CA-CB-CG	5.80	128.64	115.30
1	B	244	VAL	CB-CA-C	-5.55	100.85	111.40
1	A	278	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	341	ASP	C-N-CD	5.09	139.09	128.40
1	A	325	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5163	0	5236	106	1
1	B	5159	0	5228	461	1
2	A	4	0	6	0	0
2	B	4	0	6	0	0
All	All	10330	0	10476	565	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (565) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ILE:CD1	1:B:440:ILE:HG22	1.20	1.67
1:B:441:LEU:CD2	1:B:498:VAL:HB	1.31	1.61
1:B:426:ILE:HD13	1:B:440:ILE:CG2	1.35	1.56
1:B:441:LEU:HD23	1:B:498:VAL:CB	1.14	1.53
1:B:478:ASN:ND2	1:B:482:LYS:HZ1	1.21	1.39
1:B:260:SER:O	1:B:264:GLY:N	1.58	1.35
1:B:445:GLN:O	1:B:446:TYR:CD1	1.82	1.33
1:B:269:LEU:HD21	1:B:457:SER:CB	1.60	1.32
1:B:426:ILE:CD1	1:B:440:ILE:CG2	1.97	1.29
1:B:272:ILE:HG23	1:B:278:LEU:CD1	1.66	1.24
1:B:287:ARG:HD2	1:B:332:VAL:CG1	1.65	1.24
1:B:441:LEU:HD23	1:B:498:VAL:CG1	1.65	1.23
1:B:269:LEU:HD11	1:B:457:SER:O	1.04	1.21
1:B:285:ILE:HG12	1:B:332:VAL:HG22	1.21	1.19
1:B:287:ARG:CD	1:B:332:VAL:CG1	2.20	1.19
1:B:426:ILE:HD11	1:B:440:ILE:HG22	1.23	1.17
1:B:478:ASN:ND2	1:B:482:LYS:NZ	1.92	1.16
1:B:478:ASN:CG	1:B:482:LYS:NZ	1.99	1.16
1:B:297:ASP:CG	1:B:300:ALA:HB3	1.65	1.15
1:B:269:LEU:CD1	1:B:457:SER:O	1.93	1.15
1:B:287:ARG:HH11	1:B:332:VAL:HG11	1.11	1.13
1:B:478:ASN:CG	1:B:482:LYS:HZ2	1.53	1.11
1:B:287:ARG:CD	1:B:332:VAL:HG13	1.79	1.11
1:B:297:ASP:OD2	1:B:300:ALA:HB3	1.51	1.09
1:B:269:LEU:CD2	1:B:457:SER:OG	2.00	1.09
1:B:278:LEU:CD2	1:B:280:LYS:HD3	1.81	1.09
1:B:284:MSE:HG2	1:B:286:THR:HG23	1.29	1.08
1:B:278:LEU:HD21	1:B:280:LYS:CD	1.83	1.07
1:B:272:ILE:HG23	1:B:278:LEU:HD12	1.07	1.07
1:B:441:LEU:HG	1:B:498:VAL:HG12	1.34	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LEU:CD2	1:B:498:VAL:CB	2.05	1.05
1:B:426:ILE:HD13	1:B:440:ILE:HG21	1.14	1.05
1:B:443:ASP:OD1	1:B:445:GLN:N	1.88	1.04
1:B:246:GLN:OE1	1:B:246:GLN:N	1.91	1.04
1:B:458:LYS:NZ	1:B:458:LYS:O	1.90	1.04
1:B:285:ILE:HG12	1:B:332:VAL:CG2	1.87	1.04
1:B:269:LEU:CD2	1:B:457:SER:CB	2.35	1.03
1:B:269:LEU:HD21	1:B:457:SER:OG	1.57	1.03
1:B:279:PRO:HG2	1:B:325:LEU:HD21	1.36	1.03
1:B:287:ARG:HD2	1:B:332:VAL:HG13	1.36	1.03
1:B:307:PHE:CE1	1:B:345:LEU:HD21	1.93	1.02
1:B:278:LEU:HD21	1:B:280:LYS:HD3	1.03	1.02
1:B:287:ARG:HD2	1:B:332:VAL:HG11	1.39	1.01
1:B:269:LEU:HA	1:B:272:ILE:HD12	1.41	0.99
1:B:441:LEU:CG	1:B:498:VAL:HG12	1.93	0.99
1:B:273:VAL:HG21	1:B:457:SER:HB3	1.44	0.99
1:B:273:VAL:HG11	1:B:457:SER:HB2	1.43	0.99
1:B:441:LEU:HD21	1:B:499:SER:H	1.27	0.97
1:B:251:THR:HG22	1:B:252:LEU:H	1.30	0.96
1:B:376:LYS:HZ2	1:B:379:ILE:HD12	1.28	0.96
1:B:363:TYR:HE1	1:B:383:CYS:SG	1.88	0.95
1:B:488:HIS:HB3	1:B:491:GLU:HG2	1.47	0.95
1:B:441:LEU:HD21	1:B:499:SER:N	1.81	0.95
1:B:269:LEU:HD21	1:B:457:SER:HB2	1.46	0.94
1:B:490:THR:OG1	1:B:491:GLU:OE2	1.85	0.94
1:B:376:LYS:HA	1:B:376:LYS:NZ	1.83	0.94
1:B:272:ILE:HG22	1:B:277:PHE:HA	1.48	0.93
1:B:429:MSE:HE2	1:B:437:GLY:HA2	1.48	0.93
1:B:226:ASN:C	1:B:229:PHE:HD1	1.73	0.93
1:B:272:ILE:CG2	1:B:278:LEU:HD12	1.98	0.92
1:B:269:LEU:CD2	1:B:457:SER:HB2	1.99	0.92
1:B:441:LEU:CD2	1:B:498:VAL:CG1	2.40	0.92
1:B:430:ASP:C	1:B:430:ASP:OD1	2.06	0.92
1:B:445:GLN:O	1:B:446:TYR:HD1	1.39	0.92
1:B:426:ILE:HD12	1:B:440:ILE:HG22	1.47	0.91
1:B:287:ARG:HD3	1:B:332:VAL:CG1	1.96	0.91
1:B:434:PRO:CB	1:B:491:GLU:HG3	1.99	0.91
1:B:485:PHE:CD2	1:B:492:PHE:CD1	2.59	0.91
1:B:455:VAL:HG12	1:B:501:GLY:H	1.34	0.91
1:B:284:MSE:HG2	1:B:286:THR:CG2	2.00	0.90
1:B:297:ASP:OD1	1:B:300:ALA:CB	2.19	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:THR:HB	1:B:361:PRO:HB3	1.51	0.90
1:B:251:THR:HG22	1:B:252:LEU:N	1.88	0.89
1:B:485:PHE:CE2	1:B:500:THR:OG1	2.27	0.88
1:B:297:ASP:CG	1:B:300:ALA:CB	2.41	0.87
1:B:376:LYS:NZ	1:B:379:ILE:HD12	1.87	0.87
1:B:278:LEU:HD22	1:B:279:PRO:O	1.75	0.87
1:B:486:GLY:O	1:B:489:PRO:HD3	1.74	0.87
1:B:269:LEU:O	1:B:273:VAL:HG13	1.75	0.86
1:B:279:PRO:HB3	1:B:322:GLN:CB	2.06	0.85
1:B:226:ASN:C	1:B:229:PHE:CD1	2.33	0.85
1:B:433:GLU:O	1:B:436:LYS:HB2	1.77	0.85
1:B:478:ASN:HD21	1:B:482:LYS:HZ1	1.20	0.85
1:B:485:PHE:HD2	1:B:492:PHE:O	1.58	0.85
1:B:287:ARG:HH11	1:B:332:VAL:CG1	1.88	0.85
1:B:285:ILE:CG1	1:B:332:VAL:HG22	2.05	0.84
1:B:234:MSE:O	1:B:237:ILE:HG22	1.76	0.84
1:B:383:CYS:O	1:B:387:ILE:HG13	1.78	0.84
1:B:285:ILE:O	1:B:285:ILE:HD12	1.77	0.83
1:B:285:ILE:O	1:B:286:THR:OG1	1.96	0.83
1:B:241:LEU:O	1:B:244:VAL:HG23	1.79	0.83
1:B:453:VAL:HG11	1:B:505:LEU:HB2	1.61	0.83
1:B:430:ASP:OD1	1:B:430:ASP:O	1.96	0.83
1:B:485:PHE:CZ	1:B:500:THR:OG1	2.31	0.82
1:B:297:ASP:OD2	1:B:300:ALA:CB	2.28	0.82
1:B:434:PRO:HG2	1:B:488:HIS:CG	2.14	0.81
1:B:488:HIS:HB3	1:B:491:GLU:CG	2.10	0.81
1:B:434:PRO:HB3	1:B:491:GLU:HG3	1.62	0.81
1:B:287:ARG:NH1	1:B:332:VAL:HG11	1.94	0.80
1:A:285:ILE:HD12	1:A:287:ARG:H	1.47	0.80
1:B:225:ASP:OD1	1:B:225:ASP:N	2.10	0.79
1:B:272:ILE:CG2	1:B:278:LEU:CD1	2.55	0.79
1:B:285:ILE:CG2	1:B:329:ASN:O	2.30	0.79
1:B:441:LEU:CG	1:B:498:VAL:CG1	2.60	0.79
1:B:267:SER:HB3	1:B:396:ILE:HG13	1.66	0.77
1:B:235:ILE:O	1:B:235:ILE:HD12	1.84	0.77
1:B:244:VAL:HB	1:B:248:SER:OG	1.84	0.77
1:B:279:PRO:CB	1:B:322:GLN:HA	2.14	0.77
1:B:257:VAL:CG2	1:B:359:ASP:HA	2.14	0.77
1:A:260:SER:O	1:A:264:GLY:N	2.19	0.76
1:B:237:ILE:O	1:B:237:ILE:HD13	1.86	0.76
1:A:224:ASP:HB3	1:A:227:MSE:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:MSE:SE	1:B:284:MSE:H	2.19	0.76
1:B:377:ARG:HH21	1:B:377:ARG:HG2	1.51	0.76
1:B:441:LEU:HB3	1:B:498:VAL:HG11	1.66	0.76
1:B:388:ARG:O	1:B:421:ARG:NH2	2.18	0.76
1:B:572:PHE:O	1:B:576:GLN:NE2	2.19	0.76
1:B:308:PRO:HG3	1:B:344:ARG:HB2	1.68	0.75
1:B:443:ASP:OD1	1:B:444:ARG:N	2.19	0.75
1:B:273:VAL:HG11	1:B:457:SER:CB	2.14	0.75
1:B:363:TYR:CE1	1:B:383:CYS:SG	2.71	0.75
1:B:376:LYS:HA	1:B:376:LYS:HZ1	1.52	0.75
1:B:270:GLU:O	1:B:273:VAL:HG22	1.87	0.75
1:B:480:ASN:HA	1:B:483:ASN:OD1	1.86	0.74
1:B:229:PHE:HA	1:B:232:LYS:HG2	1.68	0.74
1:B:310:LEU:HD23	1:B:310:LEU:N	2.02	0.74
1:B:493:GLY:O	1:B:496:SER:HB3	1.86	0.74
1:B:285:ILE:HD11	1:B:287:ARG:HB2	1.68	0.74
1:B:272:ILE:HG21	1:B:277:PHE:CD1	2.24	0.73
1:B:240:LEU:N	1:B:240:LEU:HD23	2.03	0.73
1:B:226:ASN:O	1:B:229:PHE:HD1	1.71	0.73
1:B:286:THR:O	1:B:361:PRO:HG3	1.89	0.73
1:B:434:PRO:HB3	1:B:491:GLU:CG	2.18	0.73
1:B:472:ASN:HD21	1:B:475:ALA:HB3	1.52	0.73
1:B:434:PRO:HG2	1:B:488:HIS:ND1	2.04	0.73
1:A:843:VAL:O	1:A:847:ASN:HB2	1.89	0.73
1:B:455:VAL:HG12	1:B:501:GLY:N	2.02	0.72
1:B:485:PHE:CD2	1:B:492:PHE:HD1	2.07	0.72
1:B:640:THR:HG21	1:B:706:LYS:HA	1.70	0.72
1:B:269:LEU:HD21	1:B:457:SER:CA	2.19	0.72
1:B:287:ARG:HD3	1:B:332:VAL:HG13	1.61	0.72
1:B:339:THR:HG23	1:B:340:ASP:N	2.05	0.72
1:B:375:LEU:N	1:B:375:LEU:HD23	2.03	0.71
1:B:307:PHE:CE1	1:B:345:LEU:CD2	2.73	0.71
1:B:269:LEU:HD23	1:B:270:GLU:N	2.05	0.71
1:B:278:LEU:CD2	1:B:280:LYS:CD	2.54	0.71
1:B:265:LYS:O	1:B:268:VAL:HG23	1.91	0.71
1:B:454:GLY:O	1:B:500:THR:HB	1.91	0.71
1:A:642:LEU:HD22	1:A:643:GLY:H	1.55	0.70
1:B:279:PRO:HB3	1:B:322:GLN:HA	1.74	0.70
1:B:275:HIS:CG	1:B:276:GLU:H	2.09	0.70
1:B:286:THR:O	1:B:361:PRO:CG	2.40	0.70
1:B:260:SER:N	1:B:263:SER:HB3	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:PRO:HB3	1:B:322:GLN:HB2	1.71	0.70
1:B:279:PRO:O	1:B:280:LYS:HD2	1.92	0.69
1:B:878:ASP:HB3	1:B:881:VAL:HG22	1.74	0.69
1:B:285:ILE:HG13	1:B:287:ARG:CB	2.22	0.69
1:B:339:THR:HG23	1:B:340:ASP:H	1.57	0.69
1:B:690:ARG:NH1	1:B:844:GLU:OE2	2.26	0.69
1:B:285:ILE:HG13	1:B:287:ARG:H	1.56	0.69
1:B:694:THR:HG21	1:B:845:MSE:HB2	1.73	0.69
1:B:499:SER:O	1:B:500:THR:HG23	1.93	0.69
1:B:279:PRO:HB3	1:B:322:GLN:CA	2.22	0.69
1:B:286:THR:O	1:B:361:PRO:HB3	1.93	0.69
1:B:499:SER:O	1:B:500:THR:CG2	2.41	0.68
1:B:278:LEU:HB2	1:B:279:PRO:HD2	1.76	0.68
1:B:279:PRO:HG2	1:B:325:LEU:CD2	2.21	0.68
1:B:473:LEU:O	1:B:476:SER:OG	2.05	0.68
1:A:687:LEU:HD22	1:A:845:MSE:HE2	1.76	0.68
1:B:224:ASP:CG	1:B:227:MSE:HB2	2.14	0.68
1:B:231:THR:O	1:B:235:ILE:HG22	1.94	0.68
1:B:278:LEU:HD13	1:B:278:LEU:O	1.94	0.68
1:B:272:ILE:HG23	1:B:278:LEU:H	1.58	0.68
1:B:272:ILE:CG2	1:B:278:LEU:H	2.05	0.67
1:B:478:ASN:OD1	1:B:482:LYS:NZ	2.17	0.67
1:B:434:PRO:HB2	1:B:491:GLU:HG3	1.76	0.67
1:B:272:ILE:HG23	1:B:278:LEU:HD13	1.70	0.67
1:B:472:ASN:ND2	1:B:475:ALA:HB3	2.10	0.67
1:A:434:PRO:HG2	1:A:488:HIS:CG	2.30	0.66
1:B:278:LEU:CD2	1:B:280:LYS:CG	2.73	0.66
1:B:229:PHE:O	1:B:233:LYS:HG2	1.95	0.66
1:A:429:MSE:HE2	1:A:437:GLY:HA2	1.78	0.66
1:B:269:LEU:HD23	1:B:269:LEU:C	2.16	0.66
1:B:273:VAL:CG1	1:B:457:SER:HB2	2.23	0.66
1:B:279:PRO:O	1:B:280:LYS:CD	2.44	0.66
1:B:434:PRO:HB3	1:B:491:GLU:CB	2.25	0.66
1:A:863:GLU:O	1:A:867:ALA:HB3	1.96	0.66
1:B:230:ILE:O	1:B:234:MSE:HG3	1.96	0.66
1:B:272:ILE:CG2	1:B:277:PHE:HA	2.25	0.66
1:B:278:LEU:HD22	1:B:280:LYS:HG2	1.78	0.66
1:B:272:ILE:HG21	1:B:277:PHE:HD1	1.61	0.65
1:B:273:VAL:HG21	1:B:457:SER:CB	2.23	0.65
1:B:657:GLN:HE22	1:B:684:ALA:HA	1.61	0.65
1:B:269:LEU:HD11	1:B:457:SER:C	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ARG:NH2	1:B:356:SER:OG	2.30	0.65
1:A:285:ILE:HD13	1:A:332:VAL:HG22	1.78	0.64
1:A:387:ILE:O	1:A:421:ARG:NH2	2.29	0.64
1:B:257:VAL:HG22	1:B:359:ASP:HA	1.79	0.64
1:B:232:LYS:HA	1:B:235:ILE:CG2	2.28	0.64
1:B:396:ILE:HG22	1:B:425:VAL:HB	1.79	0.64
1:B:441:LEU:HD23	1:B:498:VAL:HB	0.65	0.64
1:B:434:PRO:CG	1:B:488:HIS:CG	2.81	0.64
1:B:285:ILE:HG21	1:B:329:ASN:O	1.97	0.64
1:B:297:ASP:OD1	1:B:300:ALA:HB3	1.89	0.64
1:B:242:GLN:HE22	1:B:344:ARG:HD2	1.62	0.64
1:B:456:ILE:O	1:B:481:GLU:OE2	2.16	0.64
1:B:445:GLN:C	1:B:446:TYR:CD1	2.69	0.64
1:B:278:LEU:HD21	1:B:280:LYS:CG	2.27	0.64
1:B:485:PHE:CD2	1:B:492:PHE:O	2.47	0.64
1:B:278:LEU:CD2	1:B:280:LYS:HG2	2.27	0.64
1:A:429:MSE:HE1	1:A:441:LEU:HB2	1.79	0.63
1:A:667:SER:OG	1:A:668:SER:N	2.32	0.63
1:A:578:GLN:HA	1:A:838:VAL:HG21	1.80	0.63
1:B:363:TYR:N	1:B:363:TYR:CD1	2.66	0.63
1:B:277:PHE:HD1	1:B:278:LEU:H	1.46	0.63
1:B:363:TYR:CD2	1:B:407:THR:HB	2.33	0.63
1:B:237:ILE:HD12	1:B:241:LEU:HD11	1.81	0.63
1:B:285:ILE:CD1	1:B:287:ARG:HB2	2.29	0.63
1:B:268:VAL:O	1:B:272:ILE:HG13	1.99	0.63
1:B:252:LEU:HD23	1:B:524:THR:HG21	1.81	0.63
1:A:322:GLN:O	1:A:326:THR:OG1	2.14	0.62
1:B:294:LEU:HB3	1:B:352:ILE:HD13	1.81	0.62
1:A:843:VAL:HG21	1:B:704:PRO:HA	1.80	0.62
1:B:224:ASP:OD1	1:B:227:MSE:HB2	2.00	0.62
1:B:298:PRO:O	1:B:299:GLU:HB3	1.97	0.62
1:B:491:GLU:OE2	1:B:491:GLU:N	2.33	0.62
1:B:617:ASP:N	1:B:617:ASP:OD1	2.33	0.62
1:B:272:ILE:HG12	1:B:278:LEU:HD11	1.82	0.62
1:B:526:GLU:OE1	1:B:530:ARG:NH1	2.32	0.62
1:B:441:LEU:HB3	1:B:498:VAL:CG1	2.30	0.62
1:A:308:PRO:HG3	1:A:344:ARG:HB2	1.82	0.61
1:B:287:ARG:HD3	1:B:332:VAL:HG12	1.81	0.61
1:A:524:THR:O	1:A:528:ILE:HG13	2.01	0.61
1:B:576:GLN:H	1:B:576:GLN:NE2	1.97	0.61
1:B:272:ILE:HG12	1:B:278:LEU:CD1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:MSE:HE2	1:B:284:MSE:O	2.00	0.61
1:A:249:THR:OG1	1:A:531:GLU:OE1	2.13	0.61
1:B:377:ARG:HH21	1:B:377:ARG:CG	2.14	0.61
1:B:230:ILE:HG13	1:B:904:LEU:HD11	1.83	0.61
1:B:233:LYS:N	1:B:233:LYS:HE3	2.15	0.60
1:B:376:LYS:CE	1:B:376:LYS:HA	2.30	0.60
1:B:456:ILE:HD12	1:B:457:SER:N	2.15	0.60
1:A:286:THR:HB	1:A:361:PRO:HB3	1.84	0.60
1:B:485:PHE:HA	1:B:492:PHE:HE1	1.66	0.60
1:A:258:ILE:HG22	1:A:360:LEU:HD11	1.83	0.60
1:B:277:PHE:HD1	1:B:278:LEU:N	1.99	0.60
1:B:308:PRO:HG3	1:B:344:ARG:HG3	1.83	0.60
1:B:524:THR:O	1:B:528:ILE:HG13	2.02	0.60
1:A:690:ARG:NH1	1:A:844:GLU:OE2	2.35	0.60
1:B:279:PRO:CG	1:B:325:LEU:HD21	2.22	0.60
1:B:233:LYS:HE2	1:B:233:LYS:HA	1.84	0.60
1:B:665:ASP:OD1	1:B:676:ARG:NH2	2.34	0.60
1:B:232:LYS:HG3	1:B:233:LYS:HE3	1.83	0.59
1:B:238:ARG:HA	1:B:241:LEU:HD12	1.85	0.59
1:B:363:TYR:HD1	1:B:363:TYR:N	1.99	0.59
1:B:667:SER:OG	1:B:668:SER:N	2.36	0.59
1:B:285:ILE:C	1:B:285:ILE:HD12	2.21	0.59
1:B:232:LYS:O	1:B:235:ILE:HG23	2.02	0.59
1:A:863:GLU:O	1:A:867:ALA:CB	2.51	0.59
1:B:423:ILE:HG22	1:B:450:LEU:HD13	1.84	0.59
1:A:640:THR:HG22	1:A:706:LYS:HG2	1.85	0.58
1:A:576:GLN:N	1:A:576:GLN:OE1	2.36	0.58
1:A:878:ASP:HB3	1:A:881:VAL:HG12	1.85	0.58
1:B:387:ILE:CG2	1:B:415:VAL:HG21	2.34	0.58
1:B:441:LEU:CD2	1:B:498:VAL:CA	2.81	0.58
1:B:263:SER:HA	1:B:266:SER:OG	2.03	0.58
1:B:285:ILE:HG13	1:B:287:ARG:HB3	1.84	0.58
1:B:263:SER:OG	1:B:397:SER:HA	2.03	0.58
1:B:276:GLU:HG2	1:B:277:PHE:N	2.19	0.58
1:B:454:GLY:O	1:B:500:THR:CG2	2.52	0.58
1:B:286:THR:O	1:B:361:PRO:CB	2.52	0.58
1:B:458:LYS:C	1:B:458:LYS:HZ3	1.98	0.58
1:B:574:ARG:H	1:B:575:PRO:HD2	1.67	0.58
1:B:269:LEU:HD21	1:B:457:SER:C	2.24	0.57
1:B:242:GLN:HE22	1:B:344:ARG:CD	2.16	0.57
1:B:251:THR:CG2	1:B:252:LEU:H	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:GLY:O	1:B:500:THR:CB	2.52	0.57
1:B:229:PHE:HA	1:B:232:LYS:CG	2.34	0.57
1:B:441:LEU:CD2	1:B:498:VAL:HG12	2.17	0.57
1:B:277:PHE:CD1	1:B:278:LEU:N	2.73	0.57
1:B:269:LEU:HA	1:B:272:ILE:CD1	2.27	0.57
1:A:259:GLY:HA2	1:A:408:ALA:HB2	1.87	0.57
1:B:275:HIS:H	1:B:275:HIS:CD2	2.22	0.56
1:A:665:ASP:OD1	1:A:676:ARG:NH1	2.38	0.56
1:B:255:ILE:HD11	1:B:355:LEU:HG	1.87	0.56
1:B:275:HIS:CG	1:B:276:GLU:N	2.72	0.56
1:B:610:ARG:HE	1:B:610:ARG:HA	1.70	0.56
1:B:284:MSE:N	1:B:284:MSE:SE	2.89	0.56
1:A:661:GLU:OE2	1:A:676:ARG:NH2	2.39	0.56
1:B:272:ILE:CG2	1:B:277:PHE:HD1	2.18	0.56
1:B:269:LEU:CA	1:B:272:ILE:HD12	2.27	0.55
1:B:276:GLU:OE1	1:B:303:ASP:CG	2.44	0.55
1:B:339:THR:O	1:B:340:ASP:HB3	2.06	0.55
1:B:441:LEU:HD21	1:B:498:VAL:HB	1.67	0.55
1:B:264:GLY:O	1:B:268:VAL:HG22	2.07	0.55
1:B:307:PHE:CD1	1:B:345:LEU:CD2	2.89	0.55
1:A:653:ALA:HB2	1:A:845:MSE:HE1	1.88	0.55
1:B:258:ILE:HG22	1:B:360:LEU:HD11	1.89	0.55
1:B:269:LEU:HD11	1:B:458:LYS:HB2	1.89	0.55
1:B:363:TYR:HD2	1:B:407:THR:HB	1.71	0.55
1:B:243:LYS:O	1:B:243:LYS:HG2	2.07	0.55
1:B:285:ILE:CG1	1:B:287:ARG:HB2	2.37	0.55
1:A:585:LEU:HD12	1:A:834:ALA:HB2	1.89	0.55
1:B:270:GLU:HA	1:B:273:VAL:HG22	1.87	0.55
1:B:276:GLU:OE1	1:B:303:ASP:OD1	2.25	0.55
1:B:485:PHE:HZ	1:B:500:THR:HG1	1.39	0.55
1:B:308:PRO:HG3	1:B:344:ARG:CB	2.37	0.54
1:B:436:LYS:O	1:B:440:ILE:HG13	2.07	0.54
1:A:383:CYS:O	1:A:387:ILE:HG13	2.06	0.54
1:B:297:ASP:HB3	1:B:349:SER:C	2.28	0.54
1:B:257:VAL:HG22	1:B:358:ILE:O	2.08	0.54
1:B:441:LEU:CB	1:B:498:VAL:CG1	2.86	0.54
1:A:441:LEU:HD23	1:A:498:VAL:HB	1.90	0.54
1:B:492:PHE:HD1	1:B:492:PHE:O	1.90	0.54
1:B:260:SER:H	1:B:263:SER:HB3	1.72	0.54
1:B:285:ILE:HG22	1:B:329:ASN:O	2.08	0.54
1:B:232:LYS:HA	1:B:235:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:LYS:O	1:B:512:VAL:HG23	2.08	0.54
1:A:272:ILE:HG23	1:A:277:PHE:HA	1.90	0.54
1:B:285:ILE:CG1	1:B:287:ARG:CB	2.85	0.54
1:B:376:LYS:CE	1:B:376:LYS:CA	2.86	0.54
1:A:257:VAL:HG12	1:A:394:LEU:HB3	1.90	0.53
1:A:755:MSE:HE3	1:A:790:ALA:HB1	1.90	0.53
1:B:400:ASP:OD1	1:B:400:ASP:N	2.40	0.53
1:B:237:ILE:HD11	1:B:897:VAL:HG13	1.90	0.53
1:A:360:LEU:HB2	1:A:361:PRO:HD2	1.90	0.53
1:B:754:VAL:HA	1:B:779:PHE:HE2	1.73	0.53
1:B:255:ILE:HA	1:B:392:ILE:O	2.09	0.53
1:B:287:ARG:CD	1:B:332:VAL:HG11	2.12	0.53
1:B:754:VAL:HA	1:B:779:PHE:CE2	2.43	0.53
1:B:278:LEU:HD11	1:B:280:LYS:HG3	1.91	0.53
1:B:269:LEU:HD23	1:B:457:SER:CB	2.36	0.53
1:B:529:GLN:HG2	1:B:898:LEU:HD21	1.92	0.53
1:B:528:ILE:HG23	1:B:894:LEU:HD22	1.91	0.52
1:B:749:LYS:HD2	1:B:749:LYS:H	1.73	0.52
1:A:255:ILE:HD11	1:A:355:LEU:HG	1.92	0.52
1:A:400:ASP:OD1	1:A:400:ASP:N	2.41	0.52
1:B:224:ASP:N	1:B:225:ASP:OD1	2.43	0.52
1:B:259:GLY:HA2	1:B:408:ALA:HB2	1.92	0.52
1:B:308:PRO:HD2	1:B:344:ARG:O	2.10	0.52
1:B:454:GLY:H	1:B:500:THR:HG22	1.75	0.52
1:B:339:THR:CG2	1:B:340:ASP:H	2.22	0.52
1:B:296:ASN:C	1:B:298:PRO:HD3	2.30	0.52
1:B:318:PHE:HD1	1:B:321:ILE:HD12	1.75	0.52
1:B:387:ILE:HG22	1:B:415:VAL:HG21	1.91	0.52
1:A:294:LEU:HB3	1:A:352:ILE:HD13	1.92	0.52
1:B:454:GLY:O	1:B:500:THR:HG22	2.09	0.52
1:B:444:ARG:O	1:B:447:PRO:HD3	2.09	0.51
1:B:240:LEU:CD2	1:B:240:LEU:N	2.72	0.51
1:B:279:PRO:HG3	1:B:321:ILE:HG22	1.91	0.51
1:B:775:GLY:HA2	1:B:779:PHE:O	2.10	0.51
1:A:279:PRO:HG2	1:A:325:LEU:HD21	1.93	0.51
1:B:269:LEU:HD21	1:B:457:SER:O	2.10	0.51
1:B:453:VAL:HG21	1:B:505:LEU:HD23	1.92	0.51
1:A:631:GLN:HA	1:A:631:GLN:HE21	1.75	0.51
1:B:272:ILE:HG12	1:B:280:LYS:HG3	1.93	0.51
1:B:233:LYS:CA	1:B:233:LYS:CE	2.89	0.51
1:B:454:GLY:O	1:B:455:VAL:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ARG:CG	1:B:377:ARG:NH2	2.73	0.51
1:B:382:LEU:HD12	1:B:382:LEU:C	2.30	0.51
1:B:671:LYS:N	1:B:671:LYS:HD2	2.26	0.51
1:B:339:THR:CG2	1:B:340:ASP:N	2.73	0.50
1:B:834:ALA:O	1:B:838:VAL:HB	2.10	0.50
1:B:254:SER:HB2	1:B:356:SER:O	2.11	0.50
1:A:617:ASP:OD1	1:A:617:ASP:N	2.44	0.50
1:B:376:LYS:HA	1:B:376:LYS:HZ3	1.73	0.50
1:B:381:GLU:HA	1:B:381:GLU:OE1	2.10	0.50
1:A:262:SER:O	1:A:266:SER:OG	2.29	0.50
1:B:434:PRO:HB3	1:B:491:GLU:HB2	1.94	0.50
1:A:264:GLY:HA2	1:A:267:SER:HB3	1.93	0.50
1:B:272:ILE:HG23	1:B:278:LEU:N	2.26	0.50
1:B:229:PHE:O	1:B:232:LYS:HG3	2.10	0.50
1:B:615:ILE:H	1:B:615:ILE:HD12	1.77	0.50
1:A:297:ASP:HB3	1:A:349:SER:C	2.32	0.49
1:B:817:ASN:HB3	1:B:820:TYR:HB2	1.94	0.49
1:A:255:ILE:HA	1:A:392:ILE:O	2.12	0.49
1:A:723:VAL:HG21	1:A:824:VAL:HA	1.93	0.49
1:B:265:LYS:HA	1:B:268:VAL:CG2	2.42	0.49
1:B:751:LEU:HA	1:B:754:VAL:HG12	1.94	0.49
1:A:289:PRO:HB2	1:A:342:PRO:HB3	1.95	0.49
1:B:296:ASN:HB2	1:B:354:ASP:OD2	2.13	0.49
1:A:704:PRO:HA	1:B:843:VAL:HG21	1.95	0.49
1:B:889:ARG:HG3	1:B:890:ARG:N	2.27	0.49
1:B:393:ILE:HG23	1:B:422:THR:HB	1.93	0.49
1:A:488:HIS:HB3	1:A:491:GLU:HG3	1.94	0.49
1:B:376:LYS:N	1:B:376:LYS:HE2	2.28	0.49
1:B:485:PHE:HE2	1:B:500:THR:OG1	1.89	0.49
1:A:508:LYS:O	1:A:512:VAL:HG23	2.13	0.48
1:B:477:ILE:O	1:B:477:ILE:HG22	2.12	0.48
1:B:673:PRO:HD2	1:B:877:GLU:OE1	2.13	0.48
1:B:349:SER:O	1:B:352:ILE:HG13	2.13	0.48
1:A:664:LEU:HD23	1:A:676:ARG:HG3	1.96	0.48
1:B:387:ILE:O	1:B:421:ARG:NH2	2.46	0.48
1:B:593:LEU:HD21	1:B:823:GLU:HG3	1.94	0.48
1:A:254:SER:HB2	1:A:356:SER:O	2.14	0.48
1:A:616:ILE:HD13	1:A:802:LEU:HD13	1.94	0.48
1:B:279:PRO:O	1:B:280:LYS:CG	2.62	0.48
1:B:269:LEU:HD23	1:B:457:SER:HB2	1.88	0.48
1:B:478:ASN:HD21	1:B:482:LYS:NZ	1.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:N	1:B:310:LEU:CD2	2.73	0.48
1:B:639:LEU:O	1:B:642:LEU:HD23	2.14	0.48
1:B:886:ASP:HA	1:B:889:ARG:HG2	1.95	0.48
1:B:307:PHE:CD1	1:B:345:LEU:HD21	2.40	0.47
1:A:252:LEU:HD23	1:A:524:THR:HG21	1.95	0.47
1:A:285:ILE:HD12	1:A:287:ARG:N	2.23	0.47
1:B:499:SER:C	1:B:500:THR:HG23	2.34	0.47
1:B:269:LEU:HD23	1:B:457:SER:OG	2.06	0.47
1:B:865:MSE:HB3	1:B:871:LEU:HB2	1.96	0.47
1:A:640:THR:HG21	1:A:706:LYS:HA	1.95	0.47
1:A:714:ASN:OD1	1:A:714:ASN:N	2.44	0.47
1:B:267:SER:HB2	1:B:396:ILE:CD1	2.45	0.47
1:A:596:ARG:HD2	1:A:631:GLN:HG3	1.97	0.47
1:B:278:LEU:CD2	1:B:279:PRO:O	2.57	0.47
1:B:441:LEU:CB	1:B:498:VAL:HG12	2.43	0.47
1:B:308:PRO:HG3	1:B:344:ARG:CG	2.44	0.47
1:A:607:PRO:HD3	1:A:762:ARG:HG3	1.96	0.46
1:B:472:ASN:ND2	1:B:472:ASN:O	2.47	0.46
1:A:284:MSE:H	1:A:284:MSE:SE	2.48	0.46
1:B:279:PRO:HB3	1:B:322:GLN:CG	2.45	0.46
1:B:596:ARG:HG3	1:B:635:ALA:HB2	1.97	0.46
1:B:238:ARG:CZ	1:B:356:SER:OG	2.64	0.46
1:B:377:ARG:O	1:B:380:THR:OG1	2.28	0.46
1:A:227:MSE:HA	1:A:230:ILE:HG22	1.98	0.46
1:A:599:ASN:N	1:A:599:ASN:OD1	2.48	0.46
1:A:873:LYS:O	1:A:877:GLU:HG3	2.15	0.46
1:B:285:ILE:HG12	1:B:332:VAL:HG21	1.87	0.46
1:B:275:HIS:N	1:B:275:HIS:CD2	2.84	0.46
1:B:474:LEU:HG	1:B:475:ALA:H	1.80	0.46
1:B:401:THR:HG22	1:B:402:ASP:O	2.16	0.45
1:B:454:GLY:O	1:B:455:VAL:CG1	2.65	0.45
1:B:454:GLY:N	1:B:500:THR:HG22	2.30	0.45
1:B:768:VAL:HG23	1:B:770:GLY:H	1.81	0.45
1:B:272:ILE:CG1	1:B:278:LEU:HD11	2.46	0.45
1:B:484:TYR:HE1	1:B:492:PHE:CZ	2.33	0.45
1:B:727:LEU:HD21	1:B:823:GLU:HG2	1.98	0.45
1:B:278:LEU:CD1	1:B:280:LYS:HG2	2.47	0.45
1:B:284:MSE:CG	1:B:286:THR:CG2	2.85	0.45
1:B:286:THR:HB	1:B:361:PRO:CB	2.36	0.45
1:B:576:GLN:H	1:B:576:GLN:HE21	1.60	0.45
1:A:231:THR:O	1:A:235:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ASN:O	1:B:229:PHE:CD1	2.57	0.45
1:A:234:MSE:HA	1:A:237:ILE:HG22	1.97	0.45
1:A:235:ILE:HD13	1:A:356:SER:HB2	1.98	0.45
1:A:393:ILE:HG23	1:A:422:THR:HB	1.98	0.45
1:A:754:VAL:HG21	1:A:783:LEU:HD22	1.99	0.45
1:B:694:THR:HG21	1:B:845:MSE:HE3	1.98	0.45
1:A:488:HIS:HB3	1:A:491:GLU:CG	2.46	0.45
1:B:496:SER:OG	1:B:498:VAL:HG22	2.17	0.45
1:B:664:LEU:HB3	1:B:676:ARG:NH2	2.32	0.45
1:A:233:LYS:HE3	1:A:900:LYS:HD2	1.97	0.45
1:B:308:PRO:CG	1:B:344:ARG:HG3	2.47	0.45
1:B:426:ILE:HD11	1:B:440:ILE:CG2	2.04	0.45
1:A:355:LEU:HD23	1:A:357:LEU:HD22	1.99	0.45
1:A:705:TYR:CE1	1:A:832:LYS:HD3	2.52	0.45
1:B:266:SER:HB2	1:B:427:THR:OG1	2.17	0.45
1:B:238:ARG:NE	1:B:356:SER:OG	2.50	0.45
1:A:272:ILE:HD11	1:A:280:LYS:HB2	1.99	0.44
1:B:233:LYS:N	1:B:233:LYS:CE	2.80	0.44
1:B:487:SER:OG	1:B:488:HIS:CD2	2.70	0.44
1:A:344:ARG:H	1:A:344:ARG:HG2	1.63	0.44
1:A:296:ASN:H	1:A:354:ASP:HB3	1.82	0.44
1:A:530:ARG:HD3	1:A:530:ARG:HA	1.72	0.44
1:A:664:LEU:HB3	1:A:676:ARG:NH1	2.33	0.44
1:B:344:ARG:HG2	1:B:344:ARG:H	1.56	0.44
1:B:832:LYS:O	1:B:835:GLN:HG2	2.17	0.44
1:B:246:GLN:CD	1:B:247:GLY:H	2.21	0.44
1:B:318:PHE:CD1	1:B:321:ILE:HD12	2.52	0.44
1:B:285:ILE:CG1	1:B:332:VAL:CG2	2.77	0.44
1:B:578:GLN:HA	1:B:838:VAL:HG21	1.99	0.44
1:A:285:ILE:HG12	1:A:329:ASN:O	2.17	0.44
1:B:246:GLN:CG	1:B:247:GLY:N	2.80	0.44
1:B:282:SER:HB2	1:B:283:ASN:H	1.63	0.44
1:B:272:ILE:HG13	1:B:272:ILE:H	1.64	0.44
1:B:285:ILE:HG13	1:B:287:ARG:HB2	1.98	0.44
1:B:294:LEU:HB2	1:B:355:LEU:H	1.83	0.44
1:B:269:LEU:CG	1:B:457:SER:O	2.62	0.44
1:A:275:HIS:HB2	1:A:352:ILE:HG21	2.00	0.43
1:B:278:LEU:N	1:B:278:LEU:CD1	2.80	0.43
1:B:279:PRO:CG	1:B:322:GLN:HA	2.48	0.43
1:B:429:MSE:HE2	1:B:437:GLY:CA	2.34	0.43
1:B:485:PHE:CE2	1:B:492:PHE:CD1	3.04	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:GLU:CD	1:B:748:ARG:HE	2.20	0.43
1:B:863:GLU:O	1:B:867:ALA:HB3	2.18	0.43
1:A:449:LYS:C	1:A:451:GLY:H	2.20	0.43
1:B:610:ARG:NE	1:B:610:ARG:HA	2.31	0.43
1:A:376:LYS:NZ	1:A:379:ILE:HD12	2.34	0.43
1:B:445:GLN:O	1:B:446:TYR:CG	2.60	0.43
1:B:233:LYS:HE2	1:B:233:LYS:CA	2.49	0.43
1:B:457:SER:O	1:B:458:LYS:HB2	2.18	0.43
1:B:246:GLN:HE22	1:B:890:ARG:NH1	2.17	0.43
1:B:278:LEU:HD22	1:B:280:LYS:CG	2.45	0.43
1:B:355:LEU:HD23	1:B:357:LEU:HD22	2.01	0.43
1:B:455:VAL:HG12	1:B:501:GLY:CA	2.49	0.43
1:B:458:LYS:C	1:B:458:LYS:CD	2.85	0.43
1:B:492:PHE:O	1:B:492:PHE:CD1	2.70	0.43
1:B:565:PHE:HA	1:B:663:LEU:HD21	2.00	0.43
1:A:803:ARG:HA	1:A:803:ARG:HD3	1.70	0.43
1:A:251:THR:HG22	1:A:252:LEU:H	1.84	0.43
1:A:800:LEU:O	1:A:804:ILE:HG13	2.19	0.43
1:B:853:PHE:HB3	1:B:854:PRO:HD3	2.01	0.43
1:A:507:LYS:HB2	1:A:507:LYS:HE3	1.85	0.43
1:A:837:ALA:O	1:A:841:LEU:HB2	2.17	0.43
1:B:278:LEU:CD1	1:B:280:LYS:CG	2.96	0.43
1:B:322:GLN:O	1:B:326:THR:OG1	2.14	0.43
1:B:345:LEU:HD23	1:B:345:LEU:HA	1.87	0.43
1:B:481:GLU:OE1	1:B:481:GLU:N	2.52	0.43
1:A:269:LEU:CD2	1:A:457:SER:HB2	2.49	0.43
1:A:605:LEU:HD22	1:A:606:SER:N	2.34	0.43
1:A:615:ILE:H	1:A:615:ILE:HD12	1.83	0.43
1:B:272:ILE:CG2	1:B:277:PHE:CD1	2.96	0.43
1:B:278:LEU:HD13	1:B:278:LEU:C	2.39	0.43
1:A:453:VAL:HG11	1:A:505:LEU:HB2	2.01	0.42
1:B:387:ILE:CG2	1:B:393:ILE:HD12	2.49	0.42
1:A:572:PHE:HB3	1:A:850:TYR:OH	2.19	0.42
1:B:284:MSE:SE	1:B:284:MSE:O	2.87	0.42
1:B:269:LEU:CD2	1:B:457:SER:O	2.67	0.42
1:A:528:ILE:HA	1:A:531:GLU:HG2	2.01	0.42
1:B:286:THR:CB	1:B:361:PRO:HB3	2.37	0.42
1:B:483:ASN:C	1:B:483:ASN:ND2	2.73	0.42
1:A:683:ALA:HB2	1:A:853:PHE:CE1	2.55	0.42
1:B:279:PRO:O	1:B:280:LYS:HG2	2.19	0.42
1:B:491:GLU:CD	1:B:491:GLU:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:VAL:HB	1:A:280:LYS:HB3	2.02	0.42
1:A:357:LEU:HD23	1:A:357:LEU:H	1.85	0.42
1:A:744:SER:OG	1:A:786:ARG:NH2	2.51	0.42
1:B:255:ILE:HG12	1:B:513:LEU:HD21	2.01	0.42
1:B:456:ILE:C	1:B:456:ILE:HD12	2.39	0.42
1:B:574:ARG:N	1:B:575:PRO:HD2	2.33	0.42
1:B:640:THR:HG22	1:B:706:LYS:HG2	2.01	0.42
1:A:276:GLU:HG2	1:A:277:PHE:N	2.34	0.42
1:A:387:ILE:HG22	1:A:415:VAL:HG21	2.02	0.42
1:B:297:ASP:OD1	1:B:300:ALA:HB2	2.09	0.42
1:B:496:SER:OG	1:B:498:VAL:CG2	2.68	0.42
1:A:611:GLU:N	1:A:612:PRO:HD2	2.35	0.42
1:B:285:ILE:HG22	1:B:329:ASN:CA	2.50	0.42
1:B:241:LEU:HD21	1:B:528:ILE:HD11	2.01	0.41
1:B:252:LEU:HD23	1:B:252:LEU:HA	1.89	0.41
1:B:269:LEU:HD23	1:B:270:GLU:CA	2.50	0.41
1:B:433:GLU:HA	1:B:434:PRO:HD2	1.84	0.41
1:A:244:VAL:HA	1:A:893:LEU:HD13	2.02	0.41
1:B:246:GLN:HG2	1:B:247:GLY:N	2.34	0.41
1:B:272:ILE:CG2	1:B:278:LEU:N	2.81	0.41
1:B:642:LEU:HD12	1:B:643:GLY:N	2.35	0.41
1:B:288:ARG:HA	1:B:289:PRO:HD3	1.79	0.41
1:B:672:HIS:HA	1:B:877:GLU:OE2	2.20	0.41
1:B:476:SER:OG	1:B:477:ILE:N	2.53	0.41
1:B:683:ALA:HB2	1:B:853:PHE:CE1	2.56	0.41
1:B:458:LYS:HA	1:B:458:LYS:HD2	1.97	0.41
1:B:270:GLU:C	1:B:273:VAL:HG22	2.40	0.41
1:B:456:ILE:HG23	1:B:456:ILE:O	2.21	0.41
1:A:269:LEU:HD11	1:A:457:SER:O	2.19	0.41
1:B:255:ILE:HG13	1:B:357:LEU:HA	2.03	0.41
1:A:389:GLY:O	1:A:391:ASN:N	2.48	0.41
1:B:270:GLU:CA	1:B:273:VAL:HG22	2.51	0.41
1:B:392:ILE:HD12	1:B:421:ARG:O	2.21	0.41
1:B:749:LYS:O	1:B:753:GLU:HG3	2.21	0.41
1:B:723:VAL:HG11	1:B:823:GLU:HB3	2.03	0.41
1:A:376:LYS:HZ2	1:A:376:LYS:HG3	1.76	0.41
1:A:423:ILE:HG22	1:A:450:LEU:HD13	2.02	0.40
1:B:455:VAL:CG1	1:B:501:GLY:H	2.19	0.40
1:B:832:LYS:O	1:B:836:THR:HG22	2.20	0.40
1:B:272:ILE:CG1	1:B:278:LEU:CD1	2.99	0.40
1:B:224:ASP:OD2	1:B:227:MSE:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:PHE:N	1:B:307:PHE:CD1	2.90	0.40
1:B:311:GLY:O	1:B:312:LEU:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:ARG:NH1	1:B:545:GLU:OE1[5_555]	2.17	0.03

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	652/939 (69%)	627 (96%)	25 (4%)	0	100 100
1	B	652/939 (69%)	626 (96%)	26 (4%)	0	100 100
All	All	1304/1878 (69%)	1253 (96%)	51 (4%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [\(i\)](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	564/756 (75%)	493 (87%)	71 (13%)	4 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	564/756 (75%)	459 (81%)	105 (19%)	1 10
All	All	1128/1512 (75%)	952 (84%)	176 (16%)	2 18

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	THR
1	A	237	ILE
1	A	244	VAL
1	A	251	THR
1	A	255	ILE
1	A	266	SER
1	A	269	LEU
1	A	277	PHE
1	A	278	LEU
1	A	282	SER
1	A	283	ASN
1	A	284	MSE
1	A	286	THR
1	A	287	ARG
1	A	303	ASP
1	A	320	LEU
1	A	339	THR
1	A	344	ARG
1	A	346	THR
1	A	354	ASP
1	A	357	LEU
1	A	358	ILE
1	A	376	LYS
1	A	377	ARG
1	A	382	LEU
1	A	385	LYS
1	A	386	TYR
1	A	388	ARG
1	A	393	ILE
1	A	394	LEU
1	A	396	ILE
1	A	400	ASP
1	A	402	ASP
1	A	405	ASN
1	A	412	SER
1	A	423	ILE

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Mol	Chain	Res	Type
1	A	430	ASP
1	A	431	LEU
1	A	448	LEU
1	A	458	LYS
1	A	474	LEU
1	A	481	GLU
1	A	483	ASN
1	A	490	THR
1	A	491	GLU
1	A	492	PHE
1	A	500	THR
1	A	503	MSE
1	A	600	ARG
1	A	605	LEU
1	A	610	ARG
1	A	613	ASP
1	A	617	ASP
1	A	618	LEU
1	A	631	GLN
1	A	654	SER
1	A	666	LYS
1	A	690	ARG
1	A	714	ASN
1	A	727	LEU
1	A	741	LEU
1	A	762	ARG
1	A	803	ARG
1	A	811	GLN
1	A	815	LEU
1	A	817	ASN
1	A	824	VAL
1	A	838	VAL
1	A	841	LEU
1	A	873	LYS
1	A	880	LYS
1	B	225	ASP
1	B	227	MSE
1	B	228	MSE
1	B	229	PHE
1	B	230	ILE
1	B	235	ILE
1	B	237	ILE

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Mol	Chain	Res	Type
1	B	241	LEU
1	B	243	LYS
1	B	244	VAL
1	B	255	ILE
1	B	263	SER
1	B	266	SER
1	B	268	VAL
1	B	269	LEU
1	B	272	ILE
1	B	278	LEU
1	B	282	SER
1	B	283	ASN
1	B	284	MSE
1	B	285	ILE
1	B	303	ASP
1	B	310	LEU
1	B	320	LEU
1	B	344	ARG
1	B	346	THR
1	B	348	HIS
1	B	351	ASN
1	B	354	ASP
1	B	357	LEU
1	B	358	ILE
1	B	360	LEU
1	B	363	TYR
1	B	375	LEU
1	B	376	LYS
1	B	377	ARG
1	B	378	LYS
1	B	382	LEU
1	B	383	CYS
1	B	385	LYS
1	B	386	TYR
1	B	388	ARG
1	B	393	ILE
1	B	394	LEU
1	B	396	ILE
1	B	400	ASP
1	B	402	ASP
1	B	405	ASN
1	B	407	THR

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Mol	Chain	Res	Type
1	B	412	SER
1	B	423	ILE
1	B	430	ASP
1	B	431	LEU
1	B	434	PRO
1	B	448	LEU
1	B	450	LEU
1	B	456	ILE
1	B	457	SER
1	B	458	LYS
1	B	474	LEU
1	B	479	ARG
1	B	481	GLU
1	B	482	LYS
1	B	483	ASN
1	B	491	GLU
1	B	492	PHE
1	B	498	VAL
1	B	499	SER
1	B	507	LYS
1	B	515	GLN
1	B	516	GLN
1	B	546	GLN
1	B	560	ASP
1	B	572	PHE
1	B	576	GLN
1	B	581	LEU
1	B	586	ASP
1	B	596	ARG
1	B	610	ARG
1	B	615	ILE
1	B	617	ASP
1	B	631	GLN
1	B	640	THR
1	B	641	ARG
1	B	642	LEU
1	B	647	LEU
1	B	654	SER
1	B	657	GLN
1	B	671	LYS
1	B	703	LYS
1	B	714	ASN

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Mol	Chain	Res	Type
1	B	727	LEU
1	B	749	LYS
1	B	762	ARG
1	B	768	VAL
1	B	802	LEU
1	B	811	GLN
1	B	815	LEU
1	B	818	LYS
1	B	836	THR
1	B	838	VAL
1	B	841	LEU
1	B	889	ARG
1	B	893	LEU
1	B	903	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	242	GLN
1	B	275	HIS
1	B	472	ASN
1	B	478	ASN
1	B	488	HIS
1	B	576	GLN
1	B	657	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	1001	-	3,3,3	0.47	0	2,2,2	0.34	0
2	EDO	A	1001	-	3,3,3	0.46	0	2,2,2	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	1001	-	-	0/1/1/1	-
2	EDO	A	1001	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	253:PRO	C	254:SER	N	1.13

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	648/939 (69%)	-0.30	2 (0%) 94 88	64, 116, 190, 232	2 (0%)
1	B	648/939 (69%)	0.07	32 (4%) 29 18	64, 116, 338, 374	1 (0%)
All	All	1296/1878 (69%)	-0.12	34 (2%) 56 40	64, 116, 320, 374	3 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	452	TYR	6.7
1	B	453	VAL	6.2
1	B	457	SER	5.5
1	B	428	LYS	5.0
1	B	339	THR	4.6
1	B	458	LYS	4.3
1	B	273	VAL	4.1
1	B	403	LEU	3.9
1	B	430	ASP	3.6
1	B	427	THR	3.5
1	B	451	GLY	3.5
1	B	426	ILE	3.5
1	B	424	GLY	3.5
1	B	435	GLU	3.4
1	B	487	SER	3.4
1	B	270	GLU	3.2
1	B	399	ALA	3.1
1	B	267	SER	3.1
1	B	425	VAL	3.0
1	B	441	LEU	2.7
1	B	455	VAL	2.6
1	B	259	GLY	2.5
1	A	771	ASP	2.4
1	B	397	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	402	ASP	2.4
1	B	488	HIS	2.4
1	B	400	ASP	2.3
1	B	323	LYS	2.3
1	B	456	ILE	2.2
1	A	487	SER	2.2
1	B	258	ILE	2.2
1	B	502	VAL	2.2
1	B	408	ALA	2.1
1	B	434	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	A	1001	4/4	0.72	0.70	105,105,105,105	0
2	EDO	B	1001	4/4	0.74	0.37	97,97,97,97	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.